# 1-Butanol, 3-methoxy-3-methyl-, acetate

103429-90-9	DTXSID30145852	

## **Model Performance**

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# Weighted KNN model

5-fold CV	5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.91	1.08	0.91	1.08	0.92	1.00	

#### **Model Results**

Predicted value: 8.63e-01 mmHg

Global applicability domain: Inside

Local applicability domain index: 6.65e-01

Confidence level: 5.85e-01

## Nearest Neighbors from the Training Set

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Heptanoic acid Measured: 2.34 Predicted: 6.20e-03

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Nonanoic acid Measured: 3.75e-01 Predicted: 1.91e-03

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2-Butanamine Measured: 1.02e-01 Predicted: 179

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bis(2-Chloro-1-methylethyl) ether

Measured: 3.92 Predicted: 1.62

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Tetrahydrothiophene Measured: 2.00 Predicted: 13.4